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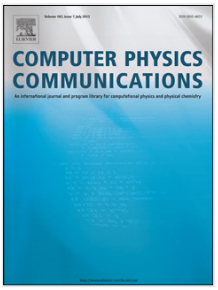


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# Exponential Type Orbitals with Generalized Hyperbolic Cosine Functions for Atomic Systems

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**Abstract**

Radial basis functions, constructed from Slater type $r^{n^*-1}e^{-\zeta r}$ and generalized exponential type $r^{n^*-1}e^{-\zeta r^{\mu}}$ functions with the generalized hyperbolic cosine type functions $\cosh_{pq}(\beta r)$ and $\cosh_{pq}(\beta r^{\mu})$, where $p$ and $q$ are arbitrary parameters, are proposed and applied to Hartree-Fock-Roothaan calculations of atomic systems. The performance of new basis functions within the minimal basis sets framework has been compared to numerical Hartree-Fock results and previous results presented by similar basis functions in literature. The results obtained by the new basis sets surpass the accuracy of existing basis sets of similar hyperbolic cosine type functions.

**Key Words:** Generalized hyperbolic cosine function, Exponential type orbital, Hartree-Fock-Roothaan calculation, Noninteger principal quantum number

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## 1. Introduction

Choosing an appropriate basis functions is one of the fundamental problems in the all quantum chemical calculations. It is well known that the natural choice of accurate and reliable basis functions in Hartree-Fock-Roothaan (HFR) method is the exponential type orbitals (ETOs). In the HFR approximation, Slater type orbitals (STOs) are the simplest analytical and suitable basis functions among the other ETOs because they represent the correct behavior of the electron-nucleus cusp condition [1] and the exponential decay at large distances [2]. Progress in the use of exponential orbitals (Slater or related type of orbitals in particular of the Sturmian type) has been lively in the last years [3-7]).

It should be also noted that the accuracy can be easily improved by increasing the number of basis functions but the cost of calculations increases significantly due to the increasing number of basis functions in HFR calculations. In order to improve the quality of basis functions and to reduce the computational cost, alternative basis functions have been